# Comparative Analysis of Qualitative Models When the Model Changes

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*An important application of the recently developed techniques in qualitative mathematical modeling is to qualitatively predict how changes in the operation of chemical units affect their behavior. Weld (1987, 1988a,b) has developed a series of comparative techniques that analyze the effect of perturbations to the parameters of a given qualitative unit model. In this article we demonstrate a system, based on the qualitative process theory of Forbus (1984), which extends comparative analysis in two ways. First, it predicts the effects of changes in the qualitative equations and in parameter values. Secondly, it compares physical descriptions, rather than comparing models directly, and builds and compares the associated models automatically.*

## Introduction

Reasoning with qualitative models of process units is an important component of intelligent systems which reason with "deep" or "first principles" knowledge of chemical plants (Dalle Molle et al., 1988; Oyeleye and Kramer, 1988; Rich and Venkatasubramanian, 1987). Comparative analysis is a branch of qualitative reasoning that predicts how changes to the inputs of a unit model affect the behavior of model parameters. It can be viewed as the qualitative analog of sensitivity or perturbation analysis of a set of equations. Comparative analysis is required for many intelligent systems. For example, in "generate and test" troubleshooting systems it is necessary to determine how hypothesized faults would change the behavior of process units (Grantham and Ungar, 1990), and in design it is necessary to compare the relative effect on process behavior of alternative design scenarios (Grantham, 1990).

Comparative analysis systems demonstrated to date are limited to analyzing the effect of changes to parameter values; the actual qualitative constraints that define the structure of the model must remain constant. Thus, although these systems can predict that an increase in the input temperature to a liquid preheater results in a higher output temperature they cannot predict that some of the liquid may vaporize. Neither can they predict that the addition of catalyst to the input would result in an exothermic reaction which would increase the exit temperature of the liquid and change its composition.

To make such deductions, comparative analysis systems must be extended in two ways. First, they must recognize that changes in a physical description may result in a change in the structure of the qualitative model, i.e., they must take on the task of modifying a model to reflect changes in process conditions rather than requiring it to be specified *a priori*. Secondly, they must be able to compare the modified and original models to determine how the structural changes affect behavior. It is, of course, still necessary to be able to analyze parameter changes within a single model.

A comparative analysis system is presented here which combines automatic model modification with model-model comparison. This enables the system to automatically determine the effects of changes in process conditions, which change the appropriate model for process units.

## Background

Several techniques have been presented that qualitatively predict how perturbations to process parameters affect the behavior of steady-state qualitative models of chemical engineering systems. For example, given a qualitative model of a heat exchanger they could predict how changes to the input temperatures, heat transfer coefficient, or fluid flow rates would affect the output temperatures. These include causal constraints (D'Ambrosio, 1989), signed digraphs (Iri et al., 1979; Umeda et al., 1980; Oyeleye and Kramer, 1988), and confluence models (Rich and Venkatasubramanian, 1987; Oyeleye and Kramer, 1988). These systems are limited in that they only consider steady-state behaviors, do not consider transitions into new qualitative states, and assume that the parameter

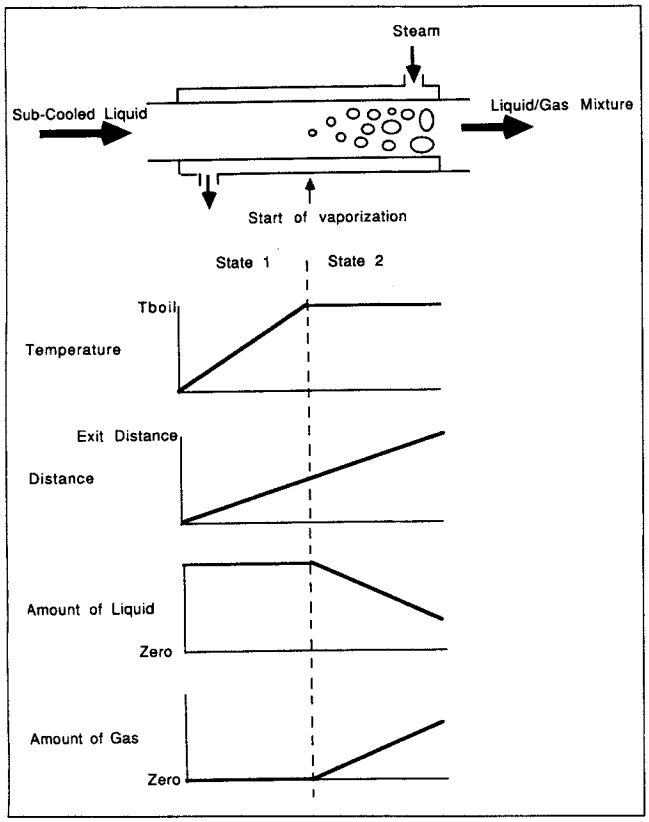


**Figure 1a. Partial vaporizer.**

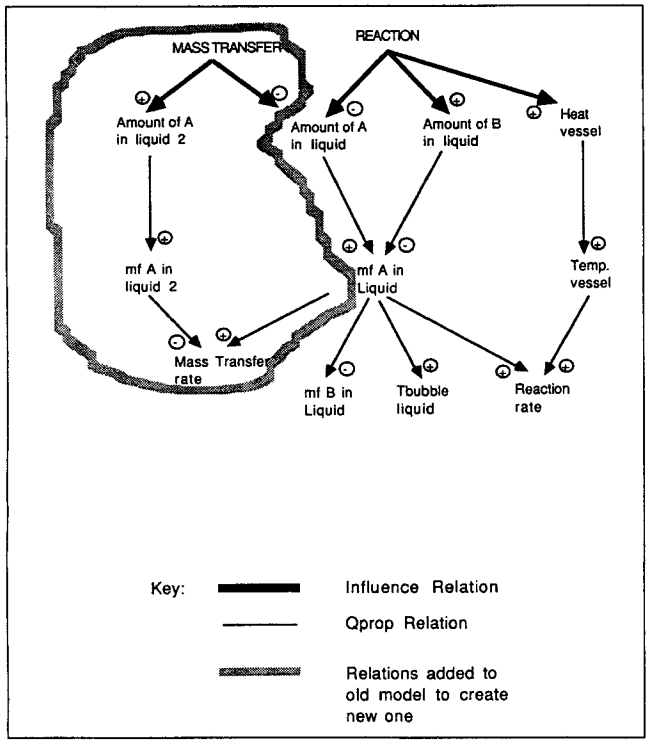


**Figure 1b. Difference between models.**

perturbations do not invalidate the supplied model. Weld (1987, 1988a,b) has developed comparative analysis techniques that predict how the dynamic behavior of a set of qualitative equations changes when the parameters of the equations are changed. His system runs on top of a QSIM envisionment (Kuipers, 1986). It can predict how changes in the starting values of parameters produce changes in interval lengths of qualitative states, changes in the values of parameters at transition points between states, and changes in the rate of change of parameters within states. In addition, because it runs on top of a QSIM envisionment it can predict changes in state transitions provided that these have been predicted *a priori* by the QSIM envisionment. However, like the signed digraph and constraint models, his system reasons directly with a specified model, which the system cannot change, but can perturb only the parameters in.

In many situations, changes in process conditions can cause changes in the structure of the model, and one wants to know how this changes the behavior of the unit. To achieve this, it is necessary for the comparative analysis system to take on the tasks of both automatically identifying how changes in physical description change the model and determining how changes to the model change the predicted behavior. In the following sections we demonstrate a comparative analysis system, based on the qualitative process theory representation of Forbus (1984), which can perform this type of reasoning.

## Overview of the System

The task of our comparative analysis system, given an initial set of process conditions and the corresponding behavior, is to determine how changes in process conditions change the behavior. These process conditions are associated with a qualitative model which is solved to obtain the behavior of the unit. This behavior is described as a sequence of *qualitative states*, the *transition* between states being characterized by a change in (qualitative) value of one or more parameters. For example, consider the behavior of an elemental volume of fluid as it passes through a partial vaporizer as shown in Figure 1. The behavior is described as passing through two qualitative states. The first state has the temperature of the liquid lower than its boiling point and increasing with increasing distance through the exchanger until it reaches its boiling point. At this point the behavior changes to another state, which consists of constant temperature vaporization, as it passes through the rest of the exchanger. This final state makes a transition when the distance along the pipe reaches the exit length. The comparative analysis system predicts the effect of changes in conditions on process behavior. Adopting the terminology of Weld, this is described in terms of a set of *relative changes* to parameter values and their derivatives. The comparative analysis system determines the relative changes at the beginning and end of each state (i.e., at each transition) and determines the change in duration of each interval (i.e., the time between transitions). There are two types of behavioral changes to consider. The first is when the behavior is altered, but proceeds through the same series of transitions. The second is when the behavior proceeds through a different series of parameter transitions.

Changes in process conditions can influence behavior via two mechanisms: by changing the value of process parameters or by changing the constraints of the model. In this article we consider only the situation where the model itself changes; parameter perturbations have already been covered by Weld.

Changes to the qualitative model arise when the process conditions are modified such that the physics or chemistry underlying the behavior is changed. This may occur in two circumstances: either when a new object is introduced into the process description (for example, addition of catalyst to a heat exchanger stream) or when a parameter makes a transition to a new qualitative value (for example, the liquid stream of a heat exchanger unexpectedly reaching its boiling point before reaching the exit).

The system comprises the following components, which will be considered in detail in the following sections:

- Mapping from changes in process conditions to changes in the model
- Comparing modified and original models
- Predicting the resultant changes in behavior (i.e., relative changes at each transition, changes to interval durations, and changes in transitions).

Behavior which consists of a single qualitative state will be presented first. We will then show how this can be extended to behavior which is described by a sequence of qualitative states.

## Terminology

Following the terminology of Kuipers (1986), the qualitative behavior of any system is defined by the values of each variable and its derivative at and between an ordered sequence of distinguished time points ($T_i$). A distinguished time point is an instant at which some variable (or its derivative) changes qualitative values. For example, the vaporizer described in the previous section is described by three distinguished time points corresponding to the time of entrance to the pipe (distance = 0), time at which vaporization first occurs (temperature = boiling point) and the time of exit from the pipe (distance = pipe length). The behavior of a variable, $q$, at any time point, $T_i$, is described in terms of a qualitative value, $QS(q, T_i)$, and the sign of its derivative, $QDIR(q, T_i)$. Similarly, the behavior of a variable over the interval between two distinguished time points, $T_i$ and $T_{i+1}$, is described by a value, $QS(q, T_i, T_{i+1})$, and a derivative, $QDIR(q, T_i, T_{i+1})$.

For example, the behavior of the temperature of an elemental volume of fluid as it passes through the vaporizer is described as follows:

| Time Point/Interval | *QDIR* Temp. | *QS* Temp. |
|---|---|---|
| $T_0$ (distance = 0) | + | 0 < Temp. < boiling pt. |
| $[T_0, T_1]$ | + | 0 < Temp. < boiling pt. |
| $T_1$ | 0 | Temp. = boiling pt. |
| $[T_1, T_2]$ | 0 | Temp. = boiling pt. |
| $T_2$ (distance = pipe-length) | 0 | Temp. = boiling pt. |

Modifying the terminology of Weld (1988), changes in the qualitative behavior of variables are defined in terms of relative changes. For example, $RC\text{-}QDIR(q, T_i, T_{i+1}) = +$ indicates that the derivative of $q$ over the interval $[T_i, T_{i+1}]$ has increased, i.e., it has experienced a positive relative change. Similarly, $RC\text{-}QS(q, T_i) = 0$ indicates that the value of $q$ at time point $T_i$ has not changed.

Let us also define the duration of an interval $[T_i, T_{i+1}]$, i.e., the time between the two consecutive time points, as $DUR(T_i, T_{i+1})$ and the relative change in duration as $RC\text{-}DUR(T_i, T_{i+1})$.

```
(Reaction ?l1)
    Individuals:          ?l1 a 2 component liquid of form (2-c-l-p A B ?c)
    Preconditions:        (contains ?c catalyst)
    QuantityConditions:   (greater-than (mf A ?l1) (rn-equil-mf A ?l1))
    Relations:            (Qprop reaction-rate (temperature ?c))
                          (Qprop reaction-rate (mf A ?l1))
                          (Qprop- reaction-rate (rn-equil-mf A ?l1))
    Influences:           (I+ (heat ?c) reaction-rate)
                          (I+ (amount-of B ?l1) reaction-rate)
                          (I- (amount-of A ?l1) reaction-rate)
```

**Figure 2a. Simplified description of the phenomenon "reaction".**

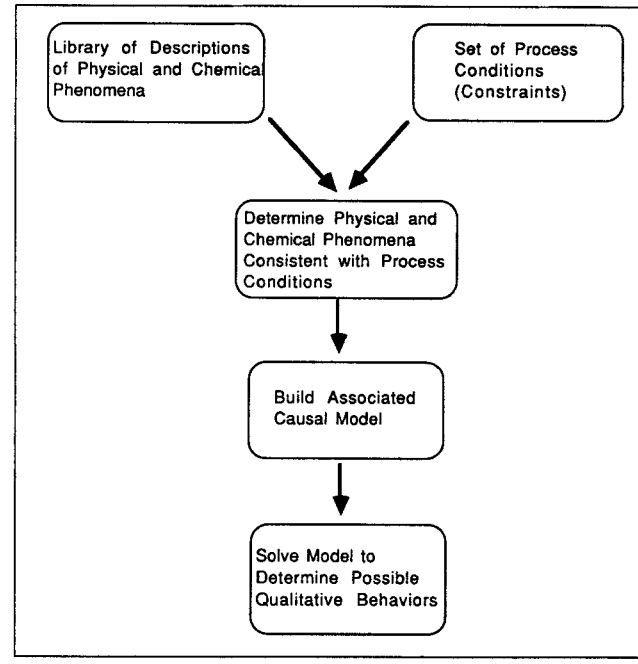


**Figure 2b. Model building and solution using qualitative process theory.**

For example, an increase in the time taken between entering the vaporizer and achieving boiling point would be described as $RC\text{-}DUR(T_0, T_1) = +$. Finally, let us define a transition variable, $TV(q, T_i)$, as a variable whose change of state is associated with the distinguished time point $T_i$. In the vaporizer example, there are two transition variables associated with the distinguished time point $T_1$: $TV$(temperature, $T_1$) and $TV$(boiling point, $T_1$).

## Single-State Behavior

### *Mapping from changes in process conditions to changes in model*

Our system is based on Forbus' qualitative process engine (QPE) (1988), which is an implementation of his qualitative process theory (QPT) (1984). This allows the definition of a set of fundamental physical and chemical phenomena (Figure 2a), which the system can use to build causal models from a physical description of the substances present and process conditions prevalent (Figure 2b). This enables the comparative analysis system to automatically change the constraints of the causal model to account for changes in process conditions.

A QPT-based description of a process unit has an explicit representation of the conditions on which the unit model was built. If a condition mentioned in either the preconditions or quantity condition field of a phenomena description is not explicitly stated in the scenario, QPE will automatically consider both situations when it is true and when it is false. Thus, the conditions associated with a unit model must contain an explicit representation of both which conditions are true and which are false to constrain the model creation mechanism of QPE to produce a single model. The effects of changes in process conditions are determined by removing the appropriate statement from the unit scenario and rerunning QPE: if a condition is to be removed, this is achieved by removing the assertion that this condition is true; if a condition is to be added, this is achieved by removing the assertion that the condition is false. QPE then automatically produces both the model associated with the original conditions together with that associated with the new conditions. These models are then compared as described in the next section.

For example, consider the effect of adding water to a reacting organic phase, such as would occur if there was a leak from the cooling coil in an organic batch reactor. The conditions associated with the original behavior are as follows:

```
(substance A) (substance B) (substance Water)
  (immiscible B Water)
(miscible A Water) (miscible A B) (container Reactor)
  (contains catalyst Reactor)
(expect A Reactor) (expect B Reactor)
  ((expect Water Reactor).)(:false)
```

and the associated phenomena identified by the computer are:

```
(2-COMPONENT-LIQUID A B Reactor)
(REACTION A B Reactor)
```

To consider the effect of adding water, the assertion

```
((expect water Reactor).)(:false)
```

is removed from the description. Then, when QPE is run, it will automatically consider both situations when water is and is not present and build the models associated with each. In addition to the original active phenomena, it identifies a new situation in which there is a second phase containing A and Water and mass transfer of A from the organic to the aqueous phase:

```
(2-COMPONENT-LIQUID A B Reactor)
(2-COMPONENT-LIQUID A Water Reactor)
(REACTION A B Reactor)
(LIQUID-LIQUID-MASS-TRANS {A B Phase}{A Water
Phase})
```

The system then builds the causal models associated with the original and new situations as shown in Figure 1b. Note that the models consist of two types of causal constraints (Forbus, 1984): influences (the thicker constraints) that relate how phenomena directly impose a change in a variable value, and qprops (the thinner constraints) that relate how changes in one variable impose a change on another variable. These models can be solved individually to determine the QDIR values of each variable over the interval $[T_i, T_{i+1}]$ associated with the models.

### *Predicting the effect of changes to the causal model*

We wish to predict the effect of model changes on the parameters of the original system. (For example, what effect does the addition of the second liquid phase have on the behavior of the original organic phase?) Specifically we wish to determine the *RC-QDIR* values for each variable over the interval with which the models are associated. A model can be thought of as specifying a set of causal paths that link active processes to variables and hence determine the behavior of the derivative of each system parameter. The comparative analysis system works by analyzing the changes in the causal paths influencing each variable caused by the changes in the constraints of the model and then propagating these changes throughout the other parameters of the model. A variable can be perturbed in one of two ways.

1. It can be perturbed directly by adding or removing a relation influencing the variable. This can be due to either a change in an influence relation or a change in a Qprop relation. Note that changes in Qprop relations will only affect a variable if another variable in the Qprop relation has a nonzero derivative.
2. It can be indirectly perturbed through a Qprop relation with a perturbed variable.

The system works out the effects of all direct changes to the model in terms of the relative changes of directly affected parameters and then propagates these relative changes to the other parameters via the causal links of the model. When more than one relation is changed, changes may perturb the parameters in competing directions. In this case, the system records all possible solutions together with the assumptions they make about which perturbation dominates. The consistency of solutions is maintained by using de Kleer's assumption-based truth maintenance system (de Kleer, 1986). The algorithm is discussed in greater detail in Appendix A.

### *Reasoning with interval durations, derivatives, and starting and end values*

Two sets of rules (analogous to those of Weld, 1988b) are used to determine how *RC-QDIR*$(q, T_i, T_{i+1})$ values and *RC-QS*$(q, T_i)$ values affect *RC-DUR*$(T_i, T_{i+1})$ and *RC-QS*$(q, T_{i+1})$: i.e., how changes to the starting value of a parameter and changes to the derivative over the interval affect the duration of the interval and the parameter values at its end.

The first set of rules analyze how relative changes in the starting value and derivative of the transistion parameters change the state duration. An example rule is:

**If** $TV(q, T_{i+1})$ and if *RC-QDIR*$(q, T_i, T_{i+1}) = +$ and if *QDIR*$(q, T_i, T_{i+1}) = +$ and if not *RC-QS*$(q, T_i) = -$ and if $TV(p, T_{i+1})$ and if not *RC-QDIR*$(p, T_i, T_{i+1}) = +$ **then** *RC-DUR*$(T_i, T_{i+1}) = -$

Note that the duration rules have to be slightly more specific than those used by Weld, because in qualitative process theory the qualitative values at which a parameter transitions may also be perturbed while in QSIM these values are fixed. Once the change in interval duration has been determined, the second set of rules determines the relative change in the end value, i.e., *RC-QS*$(q, T_{i+1})$, for all nontransitioning parameters given

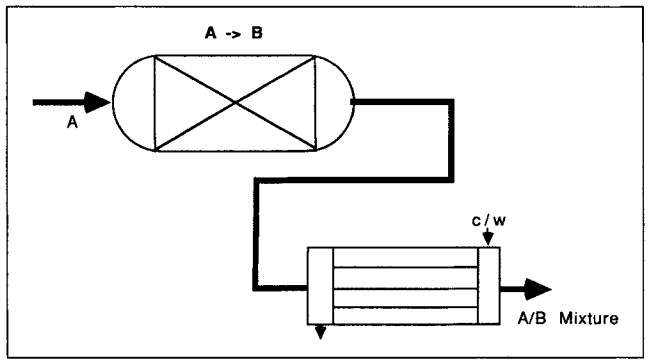


**Figure 3. Product cooler scenario.**

the changes in their starting values and derivatives. An example rule is:

**If** $QDIR(q, T_i, T_{i+1}) = +$ and if $RC\text{-}QDIR(q, T_i, T_{i+1}) = +$ and if not $RC\text{-}QS(q, T_i) = -$ and if not $RC-DUR(T_i, T_{i+1}) = -$ and if not $TV(q, T_{i+1})$ **then** $RC\text{-}QS(q, T_{i+1}) = +$

A complete set of rules, covering how all possible combinations of relative changes to starting values and derivatives affect the interval duration and end values, can be found in Appendix B, which also introduces the notation actually used in our code.

### *Case study 1: entrainment of catalyst into heat exchanger*

Consider the case of catalyst being entrained into a product cooler shown in Figure 3. The behavior of the heat exchanger

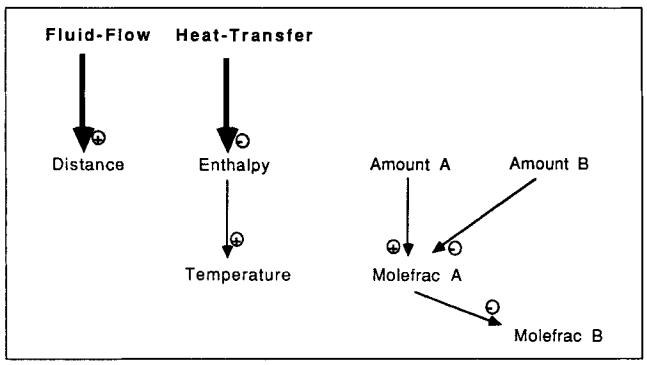


**Figure 4a. Original model (no catalyst).**

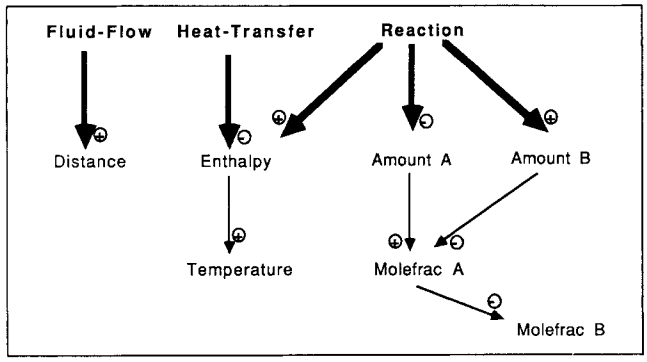


**Figure 4b. New model (entrained catalyst).**

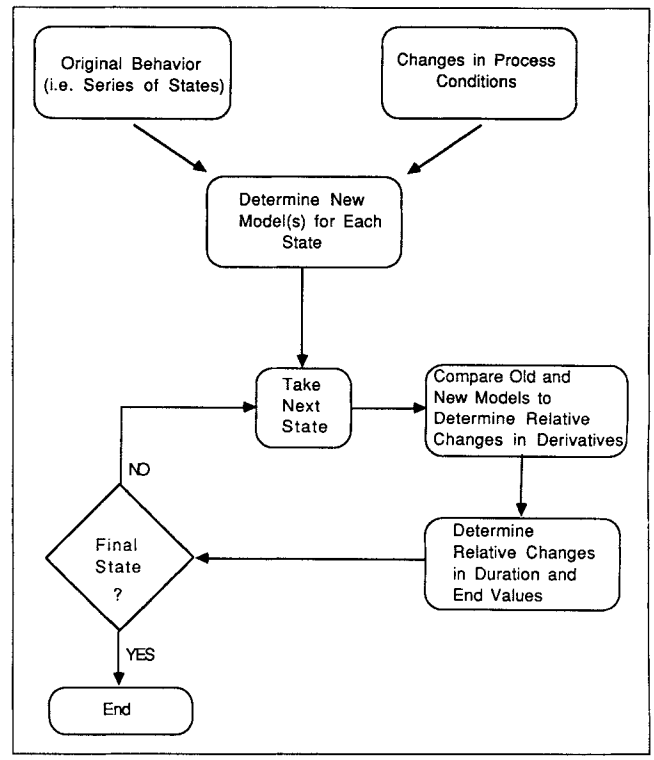


**Figure 5. Comparative analysis assuming topological equivalence.**

consists of a single-state description specified by the following conditions:

- Substance A contained in the tube side
- Substance B contained in the tube side
- A and B are miscible
- Temperature of the tube side < boiling point of A
- Temperature of the tube side < boiling point of B
- Temperature of the shell side < temperature of the tube side
- Pressure input > pressure output
- Distance < exit distance

These conditions imply the existence of three phenomena:

- The tube side contains a *two-component liquid.*
- There is *heat transfer* from the tube side to the shell side.
- There is *fluid flow* from the input to the output.

The associated model, describing the behavior of an elemental volume of fluid as it passes through the heat exchanger, is shown in Figure 4a. The solution of this model determines the signs of the parameter derivatives, as the elemental volume passes through the exchanger. The results are:

| Tube-Side Parameter | $QDIR(q, T_0, T_1)$ |
|---|---|
| Distance | + |
| Enthalpy | − |
| Temperature | − |
| Amount A | 0 |
| Amount B | 0 |
| Molefrac A | 0 |
| Molefrac B | 0 |

The behavior terminates when the distance of the elemental volume along the exchanger increases to the exit distance, i.e.,

when there is a transition from "Distance < Exit Distance" to "Distance = Exit Distance."

When the condition that catalyst is present in the heat exchanger is added to the process description, the result is to activate a fourth phenomenon, *REACTION*, which adds three new constraints to the model, as shown in Figure 4b. The effect of adding these constraints is to positively influence Amount B and Enthalpy and negatively influence Amount A. These effects are propagated through the causal links of the model to determine the relative change in the derivatives of the parameters of the system:

| Parameter | $RC\text{-}QDIR(q, T_0, T_1)$ |
|---|---|
| Distance | 0 |
| Enthalpy | + |
| Temperature | + |
| Amount A | − |
| Amount B | + |
| Molefrac A | − |
| Molefrac B | + |

Since the transition that terminates the state involves the distance parameter, which has not been affected by the changes, the state duration is unchanged. Given that the interval duration has not changed (i.e., the residence time of the elemental volume in the exchanger is the same) and that there is no relative change in the starting values, the relative changes in end-values (i.e., the values at the exit of the exchanger) are the same as the relative changes for the parameter derivatives.

Thus, the comparative analysis system has determined that the effect of catalyst being entrained into the exchanger is to produce the following changes in parameter values at the output:

| Parameter | $RC\text{-}QS(q, T_1)$ |
|---|---|
| Distance | 0 |
| Enthalpy | + |
| Temperature | + |
| Amount A | − |
| Amount B | + |
| Molefrac A | − |
| Molefrac B | + |

## Analysis of Multistate Behavior

So far we have only considered the analysis of systems whose behavior can be described by a single qualitative state. Often the dynamic behavior of a process unit will proceed through a series of qualitative states, with each state being associated with a different qualitative model. For example, fluid in a partial vaporizer will proceed through two states: a stage of heating up the subcooled liquid to its boiling point followed by a stage of liquid vaporization. In these cases there are two situations to analyze: when the system remains topologically the same (i.e., the behavior proceeds through the same series of transitions) and when the system topology changes (Weld, 1988b).

### *Comparing topologically equivalent behaviors*

Behaviors that move through the same series of transitions can be analyzed using a modification of the techniques postulated by Weld (1987, 1988b). The major difference between our system and Weld's is the incorporation of the effects of model changes in calculating relative changes of parameter derivatives. This requires that the model associated with each state in the old behavior be compared with that associated with the corresponding state of the new behavior.

To analyze the effect of changes on such multistate behavior, the following algorithm is used. For each state of the original behavior, given the changes in physical description and changes to the starting values of parameters:

1. Determine the model changes due to changes in process conditions.
2. Determine the effect of the model changes on parameter derivatives.
3. Determine the relative change in state duration.
4. Given interval duration, derivative and starting value information determine end values.
5. Repeat for each state in the sequence using the end values of previous state as starting values for the next one.

A flowchart of the system is shown in Figure 5.

### *Topologically different behaviors: transition analysis*

When analyzing for topologically different behaviors, the system determines if the perturbations to parameters could result in a different set of transitions occurring and determines the resultant change in behavior. Recall that Weld's analysis can consider only new transitions consistent with the original model. In contrast, our system can consider transitions to parameter values where new models become appropriate. This difference in ability lies in the "qualitative physics" system on which they are based. Weld's system runs on QSIM that requires *a priori* specification of the model associated with the physical system of interest. Because our system is based on the qualitative process theory, which has the ability to build its own models, it can analyze situations where the system changes to states where new models become appropriate. For example, an increased heat transfer coefficient may cause the liquid being heated in an exchanger to vaporize rather than just exit at a higher temperature.

It is possible to run our system on top of the results of a previously performed envisionment as Weld does. Because a full envisionment in the qualitative process theory covers all possible model changes, we could simply refer to the envisionment results, i.e., determine all relative changes to parameters and then look at all "child" states of the original state consistent with these perturbations. Unfortunately, the computational effort required to perform and store a full envisionment for a reasonable size plant is far too costly (Forbus and Falkenheiner, 1989). Because of this, our system performs a highly focused envisionment as part of the algorithm. This envisionment is constrained so as to only consider transitions associated with specific, prespecified parameters.

The model building and solving system works by generating all possible behaviors consistent with the supplied set of process conditions (see Forbus, 1988): the greater the number of specified conditions, the smaller the number of possible solutions. The original (design) behavior of the unit is associated with enough conditions that it is the only resulting solution. When analyzing for transitions to different qualitative states it is necessary to remove some of the original conditions. Thus,

the alternative states are generated by removing the quantity conditions associated with the variables of interest and rerunning the model builder/solver. The resulting solutions will contain the original behavior together with all alternative behaviors.

The comparative analysis comprises the following stages:

1. Determine parameters to consider for transition (specified externally).
2. Remove quantity constraints associated with these parameters from the process condition specifications.
3. Perform limited envisionment to identify possible transitions and the new behaviors associated with these.
4. Filter out transitions not consistent with relative changes.
5. Match up intervals between new and original behaviors.
6. Compare behavior between matched intervals as described earlier.

Note that in many cases the new behavior may have a different number of intervals than the original one. To match up intervals in these circumstances it is necessary to split up a single interval into a number of "pseudo intervals" to give an equal number of intervals in each sequence. We use the heuristic that the interval to be split is always the last interval of the behavior with the least number of transitions. The relative change in duration associated with pseudo intervals is determined as if it had the same transition as the state to which it is compared.

Sometimes it is better to directly compare qualitative values of the final states rather than propagating relative changes from one state to the next. For example, consider a heater with an increased heat transfer coefficient causing the heated liquid to vaporize. Splitting and comparing the behaviors result in

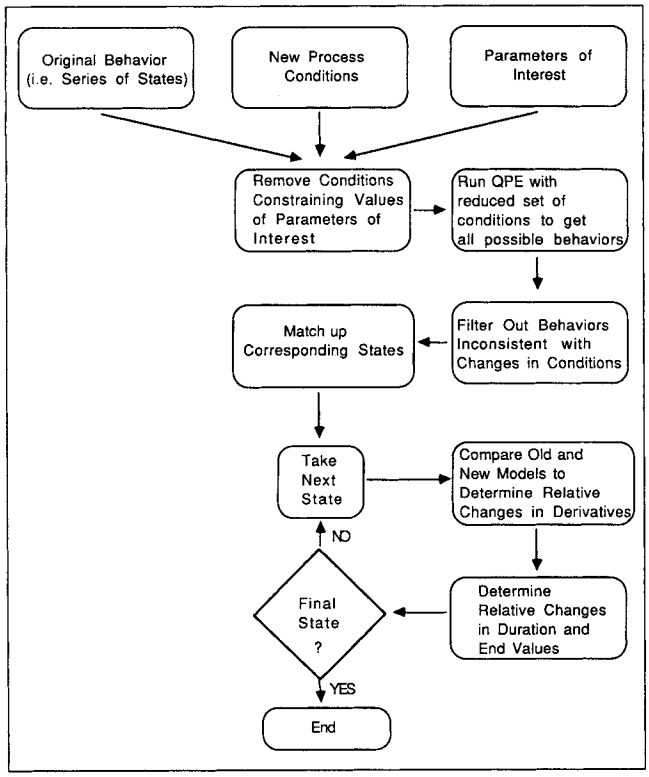


**Figure 6. Comparative analysis assuming transition to new states.**

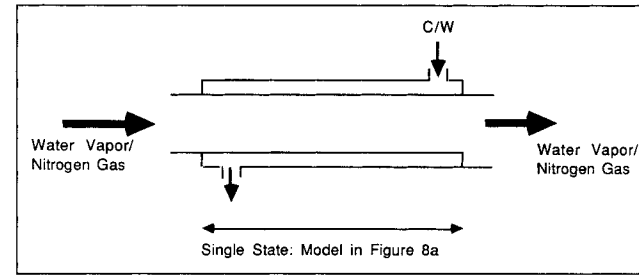


**Figure 7a. Gas cooler.**

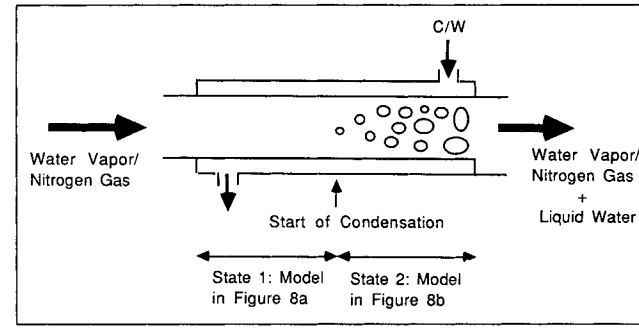


**Figure 7b. Gas cooler after increase in tube-side pressure.**

the new behavior having a higher temperature at the end of the first state; however, since it remains constant in the second state while the original behavior has its temperature increasing, it is not possible to determine which is ultimately higher! Obviously, by directly comparing qualitative states for temperature, one can determine that the new behavior has the higher exit temperature by virtue of it being at its boiling point. However, one must be careful when directly comparing final qualitative values, because these can change too. For example, if the pressure of the liquid is dropped so that it causes vaporization, the exit temperature of the new behavior may be lower than the original even though it is at its boiling point while the original is below its boiling point. The general rule followed in our system is to use matching of intervals and propagation of relative changes first and to try to resolve any resultant ambiguities using direct comparison of qualitative values providing the landmark value has not changed. A flowchart of the algorithm is shown in Figure 6.

### *Case study 2*

Consider the heat exchanger shown in Figure 7a that cools a nitrogen/water gas mixture. The behavior is described by a single qualitative state characterized by the following process conditions:

- The tube side contains nitrogen.
- The tube side contains water.
- Temperature of the tube side > dew point of water.
- Temperature of the tube side > temperature of the shell side.
- Pressure inlet > pressure outlet.
- Distance < exit distance.

These conditions activate the following phenomena:

- The tube side contains a *two-component gas*.

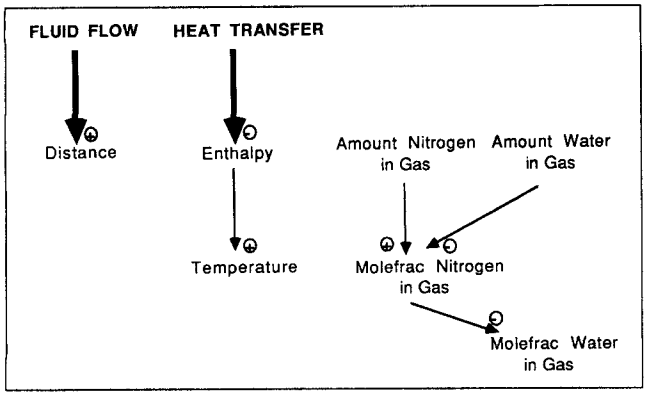


**Figure 8a. Original model ($T$ > dew point).**

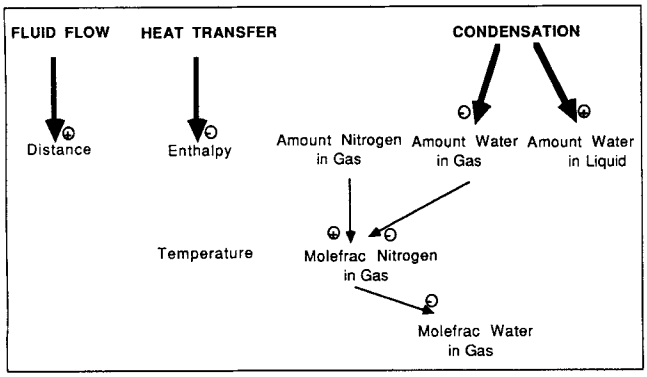


**Figure 8b. Model associated with $T$ = dew point.**

- There is *heat transfer* from the tube side to the shell side.
- There is *fluid flow* from the inlet to the outlet.

The associated causal model is shown in Figure 8a and has the solution:

| Tube-Side Parameter | $QDIR(q, T_0, T_1)$ |
|---|---|
| Enthalpy | – |
| Temperature | – |
| Distance | + |
| Amount of nitrogen | 0 |
| Amount of water | 0 |
| Molefrac of nitrogen | 0 |
| Molefrac of water | 0 |

The behavior terminates with a transition from "distance < exit distance" to "distance = exit distance."

Consider the effect of an increase in the tube-side operating pressure, i.e., a positive relative change in the starting value of pressure. In addition, specify that the system should consider only new transitions associated with temperature.

To look for transitions to new states, the conditions constraining the value of temperature are removed, i.e.,

Temperature of tube side > dew point of water
Temperature of tube side > temperature shell-side

Rerunning QPE with the above constraints removed gives the results that the original behavior could change to two other states:

Temperature of tube side = dew point of water

or

Temperature of tube side = temperature shell-side

Next, the system checks to see if either of these transitions is consistent with the relative changes associated with an increase in pressure. Firing the rules that analyze the effects of changes in starting values indicates that the increase in pressure causes an increase in the starting value for the dew point of water. Increasing the pressure does not affect the model and so all parameter derivatives have a zero relative change. Since neither the tube-side nor shell-side temperatures experience any relative changes in response to the relative increase in pressure, a transition between them cannot be a possible consequence and so is ruled out. However, the transition from the tube-side temperature to the dew point is possible because it is consistent with the increase in dew point caused by an increase in pressure.

Thus, the system has determined that, since the dew point of water has increased, the temperature may change to the dew point before the distance does to the exit distance. The result is that the behavior transits to a second state with the new condition.

Temperature of tube side = dew point water

This new condition activates an additional phenomenon in that there is now *condensation* of water from the gas to the liquid phase. The new model associated with this is shown in Figure 8b and has the following qualitative solution:

| Tube-Side Parameter | $QDIR(q, T_1, T_2)$ |
|---|---|
| Enthalpy | – |
| Temperature | 0 |
| Distance | + |
| Amount of nitrogen in gas | 0 |
| Amount of water in gas | – |
| Amount of water in liquid | + |
| Molefrac of nitrogen in gas | + |
| Molefrac of water in gas | – |

This state terminates with the transition to distance = exit distance, thus the effect of increasing the pressure is to create a two-state behavior, with the first state consisting of cooling the gas to its dew point and the second state consisting of constant temperature condensation until the exit of the tube is reached. The result of this change in operating conditions is to change the exit stream from a two-component gas to a liquid/gas mixture.

In addition to identifying this change in physical state, the comparative analysis system also determines the changes in the parameters of the original behavior by directly comparing the original and new models for each state. However, the original behavior consists of a single state while the new behavior consists of two. To obtain the same number of states in each behavior, the original state is split up into two "pseudo states," each associated with the same (original) model. Comparing the first state in both the original and new behaviors, they have the same model so there is no relative change for any derivatives. Since there is no relative change in starting values (with the exception of pressure and dew point), there is no relative change in the end values of the first state. Comparing

the models for the two final states indicates that the new model has two new constraints associated with condensation and does not have the constraint relating temperature to enthalpy. The effects of these model changes are:

| Tube-Side Parameter | *RC-QDIR*($q$, $T_1$, $T_2$) |
|---|---|
| Enthalpy | 0 |
| Temperature | + |
| Distance | 0 |
| Amount of nitrogen in gas | 0 |
| Amount of water in gas | − |
| Molefrac of nitrogen in gas | + |
| Molefrac of water in gas | − |

Since there is no relative change in the starting values of the final states, the relative changes of the end values (i.e., the exit values) are the same as in the above table for derivatives.

Thus, the comparative analysis has determined that a possible effect of increasing the operating pressure would be to induce condensation in the heat exchanger. The result of this is to produce a two-phase exit stream and to increase the exit temperature and increase the concentration of nitrogen in the exit gas phase.

## Discussion

The comparative analysis system presented, which qualitatively predicts how changes in operating conditions affect the behavior of process units, has the unique ability of predicting the effect of changes in conditions that modify the underlying physics and chemistry of the situation and hence the appropriate qualitative model. This is achieved by combining the model creation and solution capabilities of Forbus' qualitative process engine with a model-model comparison system and modified rules from Weld's differential qualitative analysis technique.

In addition to its ability to analyze situations where the model changes, our comparative analysis system differs in several aspects from that of Weld. Weld's system produces answers to problems which have only one solution. When it is asked to determine the effect of multiple, competing changes, it returns without producing an answer. In contrast, our system produces all possible solutions together with the conditions under which each is appropriate. In addition, our system can deal with situations where the landmark values (the values at which parameters transition) change, whereas Weld assumes constant landmark values. Weld's system has the advantage of being able to reparameterize and analyze behavior from different perspectives. However, we developed our comparative analysis system for use in analyzing chemical plants where behavior is almost always viewed from the perspective of time (in batch processing units) or distance (in the case of continuous processing units). As such, our system implicitly considers behaviors only in terms of these perspectives.

Our system suffers from the same limitations associated with any qualitative representation in that it tends to produce multiple solutions for even very simple problems. This gets worse as the size of the chemical plant being reasoned about increases. This ambiguity arises from the weakness of qualitative representations and manifests itself in two ways: 1) inability to order transitions; and 2) inability to resolve multiple competing tendencies.

The first problem is circumvented by allowing the system to focus only on transitions associated with prespecified parameters. Unfortunately, the system still suffers from the second problem, which in general can only be solved with additional numerical information. The number of ambiguous solutions may possibly be reduced by adopting the techniques of D'Ambrosio (1987) or Kuipers and Berleant (1988).

The examples presented are for single pieces of equipment, but our comparative analysis technique is equally applicable to the analysis of a collection of units. The relative change at the end of one piece of equipment is simply taken as the input to the following piece of equipment. Due to the tendency of the technique to produce multiple solutions, analysis of groups of units (particularly systems with recycle loops) would not be practical with the procedure presented in this article. Such an analysis, however, may be possible when combined with techniques that reduce the complexity of models by focusing on specific areas of interest. Examples of focusing systems can be found in Falkenheiner and Forbus (1988) and Grantham (1990).

Recent work by Weld (Weld, 1990) shares our goal of analyzing model changes, but differs in several important aspects. First, Weld's approximation reformulation methodology deals specifically with the situation where the new model can be transformed into the old one (or *vice versa*) by approximating a single parameter to a limit. In contrast, our system can deal with multiple changes to modeling constraints as in the condenser example where the shift to a condensing regime changes the constraints affecting both temperature and the amount of liquid. Secondly, while Weld deals with the problem of selecting alternative possible models, it still requires *a priori* specification of the qualitative models themselves. Our system has the ability to automatically build and modify models, because it is built on top of Forbus' qualitative process engine.

## Acknowledgment

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## Appendix A: Algorithm for Comparison of Two Different Causal Models

The QPT representation makes the distinction between variables that are affected by influence relations (dp variables) and those that are affected by Qprop relations (*ip* variables). *Dp* variables are affected only by the direct influence of active processes, thus it is not possible for an *ip* variable to affect a *dp* variable. This allows derivative values to be calculated in a single-pass algorithm (resolving for *dp* variables then propagating these effects to *ip* variables via Qprop relations) without encountering any loops. Unfortunately, this is not the case when performing a comparative analysis as it is possible for a perturbation in an *ip* variable to affect a *dp* variable by virtue of perturbing the associated process rate. This gives rise to a source of feedback. Thus, it is not possible to calculate the effects of model changes in a one-pass algorithm. Because of this, the system first calculates all possible changes to the rates of common processes, and hence changes to the *dp* variables influenced by these processes, and includes these when determining the relative changes of *dp* variables. The *RC-QDIR* values are calculated using the following algorithm:

1. Determine which constraints have been added or removed in moving from the original to the new model.
2. Determine the changes in the rates of common processes caused by the changes in constraints.
3. Determine the effects of adding/removing influence relations on directly influenced variables.
4. Determine the effects of adding/removing views on indirectly influenced variables.
5. Propagate these effects through the common part of the models.
6. Assert inconsistencies.

Because the possible changes in common process rates have been determined *a priori*, propagation of effects can be achieved in a single stage analogous to Forbus' QPE solution methodology.

### *Resolving for dp's*

There are two ways in which a *dp* could be influenced: being influenced by a common process whose rate has changed (as identified during step 2 above) and being affected by the addition/removal of an influence. For each variable:

1. Create two empty lists, an increase list and a decrease list.
2. For each common process with a rate change, determine its direction of effect on the variable (if any) and then insert it in the appropriate list.
3. For each addition/removal of an influence, determine its direction of effect on the variable (if any) and then insert it in the appropriate list.
4. Now we have all the positive and negative effects on the variable: if both lists are empty, set the *RC-QDIR* value to 0; if the positive list is empty (and the negative one isn't), set the *RC-QDIR* value to "$-$" and *vice versa* for an empty negative list; and if both lists are nonempty, set the *RC-QDIR* value to "$+$", "0" and "$-$", and record the conditions under which each value would be true, i.e., the positive list being greater than, equal to and less than the negative list, respectively.

### *Resolving for ips*

Again, there are two ways in which *ip* can be affected: through a Qprop relation with a changed variable and through the direct effect of the addition/removal of a Qprop constraint. *Ip* variables are resolved in an analogous manor to *dp*'s except that they must be resolved in an ordered manner such that no *ip* is resolved before the variables to which it is linked through Qprop relations are resolved.

Once all possible *RC-QDIR* values have been calculated, the system must be told what values are inconsistent. We tell the database what facts are inconsistent by running two rules on the database which create "nogoods." First, a fact cannot have more than one value at a time. Secondly, a common process must change in the same direction as its rate. (Remember we calculated changes in process rates *a priori* and used the values in the resolution steps. So we must check that the values of the rates derived during the resolve stage are consistent with initial assumptions/assertions about rate changes.)

## Appendix B: Comparative Analysis Rules

### *Definition of terms*

$\neg$(. . . .)—The statement in parentheses is not true.

**(interval ?f ?g)**—The interval over which old situation ?f and new situation ?g are being compared.

**(first-interval ?f ?g)**—The interval over which situations ?f and ?g are compared is the first interval of behavior.

**((start-value ?q) = ?dir)**—The value of quantity ?q at the start of the current interval changes in the direction ?dir. ?dir = either $-1$, 0, 1.

**((delta-dir ?q) = ?dir)**—The derivative of ?q (over the current interval) changes in the direction ?dir.

**((end-value ?q) = ?dir)**—The value of ?q at the end of the current interval changes in the direction ?dir.

**(interval-duration ?val)**—The duration of the current interval changes in the direction ?val. ?val = either decreasing, stationary, increasing.

**((reverse ?a) = ?b)**—The number ?a is negative the number ?b. ?a = either 1, $-1$.

**((int-reverse ?a) = ?b)**—The interval-duration value ?a is the reverse of the number ?b. Eg. ?a = increasing, ?b = −1.

**(pos-ind-inf-by ?q1 ?q2 ?g)**—The relation (Qprop ?q1 ?q2) appears in the model of situation ?g.

**(neg-ind-inf-by ?z ?q ?g)**—The relation (Qprop- ?q1 ?q2) appears in the model of situation ?g.

**(lower-transition-var ?q)**—The quantity ?q is involved in the transition which ends the current interval and is the transition variable which had the lowest value prior to the transition.

**(upper-transition-var ?q)**—The quantity ?q is involved in the transition which ends the current interval and is the transition variable which had the highest value prior to the transition.

**((s (d ?q)) = ?dir)**—The value of the quantity ?q is changing in the direction ?dir over the current interval. (Not to be confused with the change in derivative which is "delta-dir").

**(next-interval ?f ?g ?u ?i)**—The interval over which situations ?f and ?g are compared is immediately followed by the interval over which ?u and ?i are being compared.

Note that (lower-transition-var ?q), (upper-transition-var ?q) and (s (d ?q)) all refer to the new situation being compared. This distinction is required because the old and new situations do not necessarily have the same quantity behaviors or terminating transitions.

### *Rules*

For the first interval duration only, propagate relative changes in start values to other start values. Limited to only one input change in starting value of first interval duration.

IF Over (interval ?f ?g):
(first-interval ?f ?g)
((start-value ?q) = ?v)
¬(equal ?v 0)
(quantity ?z)
(pos-ind-inf-by ?z ?q ?g)
THEN
((start-value ?z) = ?v)

IF Over (interval ?f ?g):
(first-interval ?f ?g)
((start-value ?q) = ?v)
¬(equal ?v 0)
(quantity ?z)
(neg-ind-inf-by ?z ?q ?g)
((reverse ?v) = ?w)
THEN
((start-value ?z) = ?w)

Determine change in interval duration lengths and end-values of transition parameters. These rules assume transition variables are not moving in the same direction.

IF Over (interval ?f ?g):
(lower-transition-var ?x)
(upper-transition-var ?y)
((s (d ?x)) = ?z)
((s (d ?y)) = ?p)
¬(equal ?z ?p)
¬((delta-dir ?x) = 1)
¬((delta-dir ?y) = −1)
¬((start-value ?x) = 1)
¬((start-value ?y) = −1)
(or((delta-dir ?x) = −1)((start-value ?x) = −1))
THEN
(interval-duration increase)

IF Over (interval ?f ?g):
(lower-transition-var ?x)
(upper-transition-var ?y)
((s (d ?x)) = ?z)
((s (d ?y)) = ?p)
¬(equal ?z ?p)
¬((delta-dir ?x) = −1)
¬((delta-dir ?y) = 1)
¬((start-value ?x) = −1)
¬((start-value ?y) = 1)
(or ((delta-dir ?x) = 1)((start-value ?x) = 1))
THEN
(interval-duration decrease)

IF Over (interval ?f ?g):
(lower-transition-var ?x)
(upper-transition-var ?y)
((delta-dir ?x) = 0)
((delta-dir ?y) = 0)
((start-value ?x) = 0)
((start-value ?y) = 0)
THEN
(interval-duration stationary)
AND
((end-value ?x) = 0)
AND
((end-value ?y) = 0)

IF Over (interval ?f ?g):
(lower-transition-var ?x)
(upper-transition-var ?y)
((s (d ?x)) = ?z)
((s (d ?y)) = ?p)
¬(equal ?z ?p)
¬((delta-dir ?x) = −1)
¬((delta-dir ?y) = 1)
¬((start-value ?x) = −1)
¬((start-value ?y) = 1)
(or ((delta-dir ?y) = −1)((start-value ?y) = −1))
THEN
(interval-duration decrease)

IF Over (interval ?f ?g):
(lower-transition-var ?x)
(upper-transition-var ?y)
((s (d ?x)) = ?z)
((s (d ?y)) = ?p)
¬(equal ?z ?p)
¬((delta-dir ?x) = 1)
¬((delta-dir ?y) = −1)
¬((start-value ?x) = 1)
¬((start-value ?y) = −1)
(or ((delta-dir ?y) = 1)((start-value ?y) = 1))
THEN
(interval-duration increase)

Rule for when we get competing changes in transition variables/start-values giving 3 possibilities for internal change

IF Over (interval ?f ?g):
(upper-transition-var ?x)
((start-value ?x) = ?y)
((delta-dir ?x) = ?b)

(lower-transition-var ?n)
((start-value ?n) = ?o)
((delta-dir ?n) = ?p)
(or ((reverse ?y) = ?b)((reverse ?y) = ?p)((reverse ?y) = ?o)
((reverse ?b) = ?p)((reverse ?b) = ?o)((reverse ?p) = ?o))
THEN EITHER
(interval-duration stationary)
OR
(interval-duration increase)
OR
(interval-duration decrease)

End-values for transition parameters

IF Over (interval ?f ?g):
(transition-var ?x)
((s (d ?x)) = 0)
(transition-var ?y)
((delta-dir ?x) = 0)
((start-value ?x) = 0)
THEN
((end-value ?y) = 0)
AND
((end-value ?x) = 0)

IF Over (interval ?f ?g):
(lower-transition-var ?x)
(upper-transition-var ?y)
((delta-dir ?y) = ?p)
((start-value ?y) = ?q)
((delta-dir ?x) = ?a)
((start-value ?x) = ?b)
(or (equal ?p − 1)(equal ?q − 1)
(or (equal ?a − 1)(equal ?b − 1))
¬(or (equal ?a 1)(equal ?b 1))
¬(or (equal ?p 1)(equal ?1))
THEN
((end-value ?x) = − 1)
AND
((end-value ?y) = − 1)

IF Over (interval ?f ?g):
(lower-transition-var ?x)
(upper-transition-var ?y)
((delta-dir ?y) = ?p)
((start-value ?y) = ?q)
((delta-dir ?x) = ?a)
((start-value ?x) = ?b)
(or (equal ?p 1)(equal ?q 1))
(or (equal ?a 1)(equal ?b 1))
¬(or (equal ?a − 1)(equal ?b − 1))
¬(or (equal ?p − 1)(equal ? − 1))
THEN
((end-value ?x) = 1)
AND
((end-value ?y) = 1)

IF Over (interval ?f ?g):
(lower-transition-var ?x)
(upper-transition-var ?y)
((delta-dir ?y) = ?p)
((start-value ?y) = ?q)
((delta-dir ?x) = ?a)
((start-value ?x) = ?b)
¬(and (equal ?a 0)(equal ?b 0))
¬(and (equal ?x 0)(equal ?y 0))
(or ((reverse ?p)?a)((reverse ?p)?b)((reverse ?q)?a)((reverse ?q)?b)
((reverse ?a)?b)((reverse ?p)?q))
THEN EITHER
((end-value ?x) = 1)
AND
((end-value ?y) = 1)
OR
(end-value ?x) = − 1)
AND
((end-value ?y) = − 1)
OR
((end-value ?x) = 0)
AND
((end-value ?y) = 0)

Effects of interval-duration changes on other parameters

IF Over (interval ?f ?g):
(interval-duration decrease)
(quantity ?x)
(transition-var ?u)
¬(equal ?x ?u)
((s (d ?x)) = ?y)
((start-value ?x) = ?w)
¬(equal ?w ?y)
((delta-dir ?x) = ?e)
¬(equal ?e ?y)
((reverse ?y) = ?z)
THEN
((end-value ?x) = ?z)

IF Over (interval ?f ?g):
(interval-duration increase)
(quantity ?x)
(transition-var ?u)
¬(equal ?x ?u)
((s (d ?x)) = ?y)
((reverse ?y) = ?z)
((delta-dir ?x) = ?e)
¬(equal ?e ?z)
((start-value ?x) = ?w)
¬(equal ?w ?z)
THEN
((end-value ?x) = ?y)

IF Over (interval ?f ?g):
(interval-duration stationary)
(quantity ?x)
(transition-var ?u)
¬(equal ?x ?u)
((delta-dir ?x) = ?z)
((reverse ?z) = ?y)
((start-value ?x) = ?e)
¬(equal ?e ?y)
THEN
((end-value ?x) = ?z)

IF Over (interval ?f ?g):
(interval-duration stationary)
(quantity ?x)
(transition-var ?u)
¬(equal ?x ?u)
((start-value ?x) = ?z)

((reverse ?z) = ?y)
((delta-dir ?x) = ?e)
¬(equal ?e ?y)
THEN
((end-value ?x) = ?z)

IF Over (interval ?f ?g):
(interval-duration stationary)
(quantity ?x)
((delta-dir ?x) = 0)
((start-value ?x) = 0)
THEN
((end-value ?x) = 0)

Rules for situations when get multiple possible outcomes

IF Over (interval ?f ?g):
(quantity ?x)
((delta-dir ?x) = ?a)
((start-value ?x) = ?b)
((reverse ?a) = ?b)
THEN EITHER
((end-value ?x) = 0)
OR
((end-value ?x) = 1)
OR
((end-value ?x) = −1)

IF Over (interval ?f ?g):
(quantity ?x)
(interval-duration ?y)
((start-value ?x) = ?b)
((int-reverse ?y) = ?b)
THEN EITHER
((end-value ?x) = 0)
OR
((end-value ?x) = 1)
OR
((end-value ?x) = −1)

IF Over (interval ?f ?g):
(quantity ?x)
(interval-duration ?y)
((delta-dir ?x) = ?b)
(int-reverse ?y) = ?b)
THEN EITHER
((end-value ?x) = 0)
OR
((end-value ?x) = 1)
OR
((end-value ?x) = −1)

Rule that states that end-values of previous interval are start-values of next.

IF Over (interval ?f ?g):
(next-interval ?f ?g ?u ?i)
((end-value ?x) = ?v)
THEN
((start-value ?x) = ?v) Over (interval ?u ?i)

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